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MICHIGAN STATE UNIV EAST LANSING DEPT OF CHEMISTRY
PHOTOIONIZATION STUDIES OF MOLECULAR DYNAMICS AND ENERGETICS.(U)
JUL 79 G E LEROI

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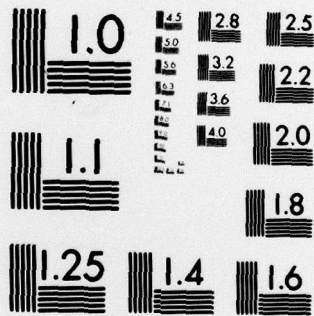
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6 Photoionization Studies of Molecular Dynamics and Energetics

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"Photoionization Studies of Molecular Dynamics and Energetics"

(Final Technical Report)

The primary scientific accomplishment during the contractual period was the completion of a sophisticated, computer-controlled photoionization mass spectrometric instrument which was designed in our laboratory. Photoionization efficiency curves for parent and daughter ions of the chlorofluoromethanes, of acetonitrile and perdeuteroacetonitrile, and preliminary curves for several other molecules of aeronomical interest, were obtained. The potentiality of the instrumentation to study ion-molecule reactions was also successfully explored.

Technical Report No. 1, dated 24 February 1978 and entitled: "The Design and Operation of an Automated, High-Efficiency Photoionization Mass Spectrometer", describes in extensive detail the design philosophy and the various components comprising the apparatus, as well as the computer-related hardware and software developed for its efficient operation. Two publications arising from this work have appeared in the open literature; two more papers will be submitted for publication shortly. In addition, at least two manuscripts describing the scientific results obtained from the data gathered by the photoionization mass spectrometer will be submitted in the future. Aspects of this project were also described at several national meetings.

Three graduate students completed their dissertation research under partial support of this contract. Their theses are listed in the bibliography of publications and presentations which follows:

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Bibliography

I. Ph.D. Theses

1. Edward J. Darland (1978)
"The Design and Operation of an Automated, High-Efficiency Photoionization Mass Spectrometer"
2. Gary W. Ray (1978)
"A Photoionization Mass Spectrometric Study of Acetonitrile and Acetonitrile-d₃"
3. David M. Rider (1979)
"Photoionization Mass Spectrometry. Studies of Substituted Methanes: CH₃CN, CD₃CN, CFC₃, CF₂Cl₂ and CF₃Cl"

II. Contributed Papers at National Meetings

1. "A Computer-Controlled Vacuum-Ultraviolet Photoionization Mass Spectrometer"
E. J. Darland, G. E. Leroi, G. W. Ray, F. P. Tully and C. G. Enke,
Paper No. 234, 27th Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy, Cleveland, 1-5 May 1976.
2. "Photoionization of Halocarbons", F. P. Tully, E. J. Darland, G. W. Ray, P. L. Kronebusch, C. G. Enke and G. E. Leroi, Paper O-9, 24th Annual Conference on Mass Spectrometry and Allied Topics, San Diego, 9-13 May 1976.
3. "A Photoionization Mass Spectrometric Study of Acetonitrile and Acetonitrile-d₃". G. W. Ray, E. J. Darland, C. G. Enke, and G. E. Leroi, Paper A-7, 25th Annual Conference on Mass Spectrometry and Allied Topics, Washington, D. C., 30 May-3 June 1977.

III. Publications

1. "Pulse (Photon) Counting: Determination of Optimum Measurement System Parameters". E. J. Darland, G. E. Leroi, and C. G. Enke, Anal. Chem. 51, 240 (1979).
2. "Pulse (Photon) Counting: A High-Speed, Direct Current-Coupled Pulse Counter". E. J. Darland, J. E. Hornshuh, C. G. Enke, and G. E. Leroi, Anal. Chem. 51, 245 (1979).
3. "A Computer-Controlled High-Efficiency Photoionization Mass Spectrometer". E. J. Darland, D. M. Rider, F. P. Tully, C. G. Enke, and G. E. Leroi, to be submitted to the International Journal of Mass Spectrometry and Ion Physics.
4. "Maximum Efficiency Pulse Counting in Computerized Instrumentation". E. J. Darland, C. G. Enke and G. E. Leroi, to be submitted to Analytical Chemistry.

Personnel

<u>Name</u>	<u>Status</u>	<u>Current Position</u>
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